Forbidden X-Ray Wavefields of Three-Beam Bragg Reflections From Thick Crystals

X. Huang and M. Dudley (SUNY, Stony Brook)

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Introduction: Multiple (*N*)-beam X-ray diffraction has recently attracted renewed attention due to its applications in solving the phase problem and in analyzing X-ray polarization states Compared with two-beam diffraction, *N*-beam diffraction involves a much more complicated scattering process. Although the diffracted intensities from this process can be computed using well-developed computational algorithms, the physical aspects related to the scattering process are usually hidden in the automated computation procedures, which make it difficult to obtain a clear understanding of the dynamical diffraction mechanisms. The purpose of our work is to provide a direct picture of the diffraction process for the commonly used three-beam diffraction. We focus on the main properties of Bragg-case diffraction from semi-infinite crystals since this geometry exhibits a number of interesting phenomena similar to the well-known properties of two-beam diffraction, such as forbidden wavefields, extinction, and total reflection. Our calculations display explicitly the transition between two- and three-beam cases and the similar excitation states of tiepoints on the dispersion surface. The differences between the thick- and thin-crystal diffraction models.

Results: In our theoretical work,[1] a detailed analysis of three-beam diffraction dispersion surface (Fig. 1) is performed to study the forbidden wavefields of thick-crystal Bragg reflections. From the asymptotic transition between two- and three-beam diffraction, it is found that the excitation state of each wavefield in thick-crystal can be accurately determined with the two-beam criterion. Consequently, Bragg-case three-beam diffraction from thick crystals is either a four-mode diffraction process for the Bragg-Laue geometry or a two-mode process for the Bragg-Bragg geometry, and the amplitudes of the excited wavefields can be completely determined by the entrance boundary conditions. This is clearly in contrast to the well-studied thin-crystal diffraction model, which is always a six-mode diffraction process. Based on this picture, the intrinsic mechanisms underlying three-beam Bragg reflections are clearly illustrated.

References: [1] X. R. Huang, M. Dudley, J. Y. Zhao, Acta Cryst. 2001 - in print.

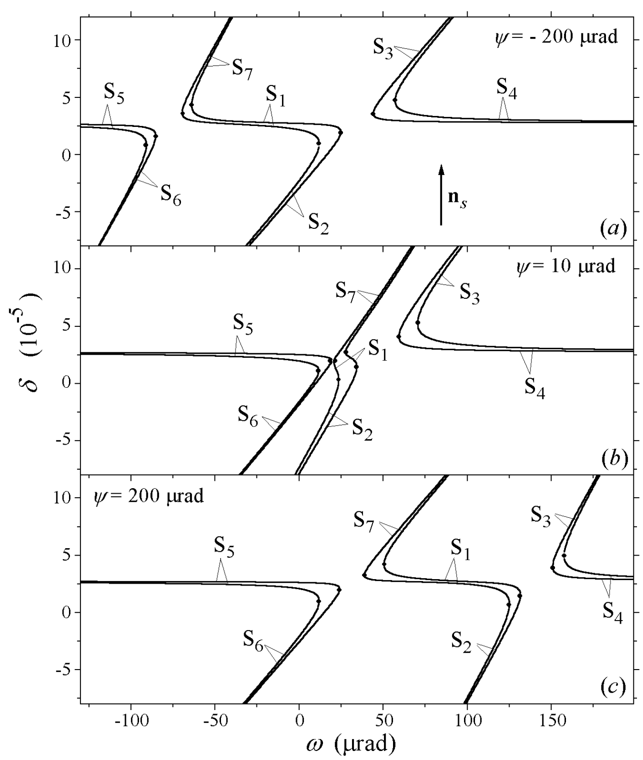

Figure 1. Evolution of the dispersion surface sections for different azimuthal angle ψ for three-beam Bragg-Bragg diffraction.

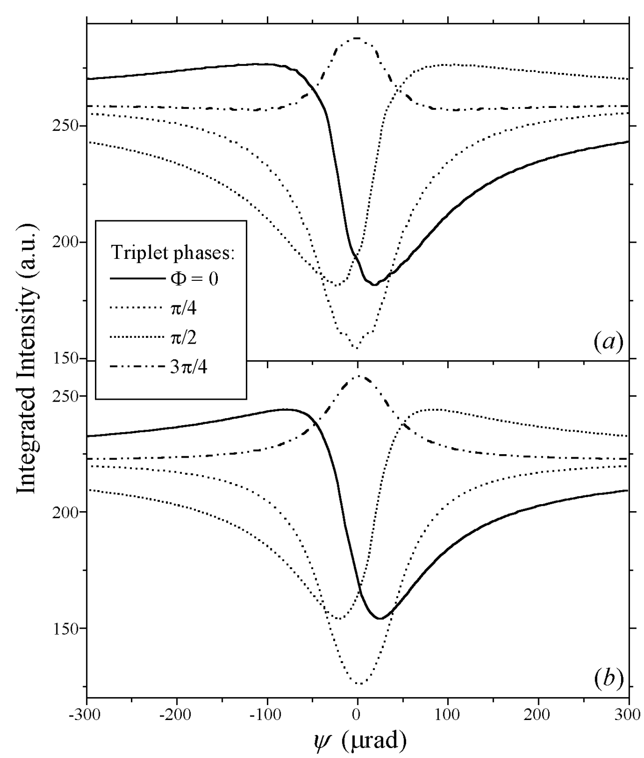

Figure 2. Interference profiles of three-beam Bragg-Bragg diffraction for four representative triplet phases Φ. (a) Thin-crystal case, six-mode diffraction. (b) Semi-infinite-crystal case, two-mode diffraction with four forbidden wavefields.